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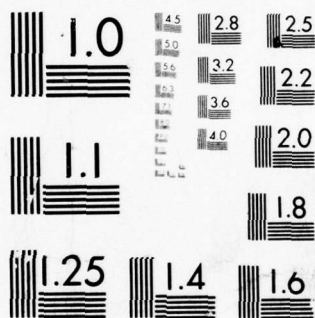   JUL 76   G PASK   F44620-76-C-0003
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Computer administered tests for cognitive style, Creativity in design Objective analysis of design process, Educational simulator, Chemical Reaction Kinetics.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The report deals with: (A) The specification of an electronics design project, which is to be used as an experimental task in a series of experiments intended to exteriorize various aspects of cognitive style and creativity in design; (B) The development of computer administered pretests and post-tests for cognitive style; (C) The overall experimental plan, including arrangements for training student designers. →(over)

and (3)

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continuation of Block no 20- Abstract

The main body of the report concerns the experimental design project. *& whose*
The project is divided into two separate, but related, design tasks.
The overall goal ~~of the project~~ is the design of a (programmable) ed-
ucational simulator for use in teaching chemical reaction kinetics.

The first design task involves the simulation of macroscopic relation-
ships (overall energy changes and reaction rate equations). •The second
task is the design of a simulator to illustrate microscopic principles
(mechanisms of molecular interaction) and should include one or more
of the first task simulators as subsystems.

The first design task is to be carried out on an individual basis, the
second task by teams of designers. The team design work in expected
to yield valuable data concerning communication between designers.•

The techniques to be used for the objective analysis of designer
behaviour. The information obtainable from computer administered
pre and post, tests for cognitive style, and some questions of design
training are discussed in shorter sections of the report.

Progress Report 3.

Contract No: F44620-76-C-0003

1st February 1976 to 30th April 1976

Principal Investigator: Gordon Pask

Submitted by:
System Research Ltd
2 Richmond Hill
Richmond
Surrey
England

Dated: July 1976

Contractor's signature ....

Progress Report 3:

Contract No : F44620-76-0-0003

Index

1.   Introduction

1.1.   Status

The first three phases of the original research objectives* have been completed. These were :

(a) Preparation of background material.
(b) Building up necessary interface equipment.
(c) Program Writing.

Phases (a) and (b) include specification of a design project which meets the experimental requirements and is acceptable (as judged by interview and discussion) to the subject population. The subject population includes both experienced designers (referred to as Group A subjects) and student designers (referred to as Group B subjects).

Phase (c) includes the development of programs for administering a pretest and a matched post test for learning style and other aspects of cognition. The rationale of such tests (especially the "Spy Ring History Test") is discussed in Research Note No 1. "Spy Ring History Test" submitted June 1976.

1.2.   Summary of Work Done

The main achievements during the last quarter are reported in Section 2 and Section 3. These Sections describe a design project which is likely to exteriorise subjects' creative activity. The project is apparently acceptable as a realistic design problem, both to Group A subjects (experienced designers) and Group B subjects (student designers).

It is convenient to divide the design project into two tasks.

*As set out in the table of Section 2.6 (page 12) of the original proposal(which appears as Appendix A to the Proposal for continuation of Contract No. F44620-76-0-0003, submitted January 1976 and assigned control number EOARD-76-036) hereinafter referred to as "the proposal"

The first task differs from the second in that the first design task is to be undertaken individually, whereas the second task is to be undertaken by teams of 4 or 5 subjects. The team design work is included in order to encourage verbal discussion and to elicit the communication data referred to in the Proposal*. Both the first and second design tasks have components (i), (ii), (iii), of the Proposal Section 2 (a), the second task also involves components (iv), (v). Both design tasks involve educational simulators for use in teaching chemical reaction kinetics.

Section 2 describes the first experimental design task which is to be performed individually.

Section 3 contains a brief account of the second experimental task which is to be attempted by teams of subjects.

Section 4 describes the computer administration of the Pre-test (the "Spy Ring History Test") and the post test, for which outline flow charts were shown in Progress Report No 2, March 1976. Emphasis is placed upon procedures, now programmed, for objectively calibrating subjects' "degree of belief" responses, for analysing their behaviour and for estimating individual learning rate (during the initial part of the test). This data may either be used "off line", by the experimenter, or with minor refinements in the programs, for "on line" adaptive administration of the tests for learning style.

Section 5 is an outline discussion of the training arrangements for student designers. (Group B subjects).

Section 6 reviews the experimental design including certain alternatives that are open at various stages.

* Proposal, Appendix A, Section 2.5. item 5.

1.3.   Preliminary Discussion of Design Task

The first task involves the design of a network to solve the differential equations governing the concentration changes in a 2 reactant, 2 product chemical reaction. The simulation basically involves 4 integrations, together with various non-linear (multiplicative) interactions and feedback regulation to impose "constant temperature" and "constant concentration" conditions. The task is open ended and can give rise to many neat and innovative designs involving compromise and some contextual reasoning in the area of general scientific knowledge as well as electronics.

The second task, also a simulator design, is much more difficult and can probably only be carried out effectively, within a reasonable interval, by a team of designers. The design necessarily incorporates, as a subsystem, a simulator of the kind produced as a solution to the first task.

The requirement, in the second task, is to simulate a chain, or series, of reaction stages ; the "activated complex" reaction model being a special case for this type of simulation. It is necessary to display the mechanism of energy transfer between reacting molecules at a microscopic rather than at a molar level (as in the first simulation). The second simulation should, therefore, rationalise for the student the otherwise arbitrary assignment of constants and parameters in the first simulation.

The specification of the second task is deliberately less firm than the first. It would be possible, for example, to terminate the second task at the point where a simulator for a reaction chain is designed, or at a point where the special case of "activated complex" theory is simulated, or, as outlined here, with the design for a simulator displaying detailed molecular mechanisms of energy transfer. It seems prudent to reserve the possibility of continuing the second design task for as long as practicable, provided it continues to yield interesting data, and the second task is specified with this option in view.

2.   A Description of the First Design Task

An outline solution to the first design task is charted in Fig 1. It is shown to provide an overview, and will not be accessible to either Group A or Group B subjects, though several features of the specification brief are indicative of this layout.

It is desirable to "over design" rather than "under design" the system and to incorporate a facility for restricting the simulation behaviour by programmed information.   The outline design of Fig 1 allows a great deal of latitude in the choice of methods and components, for example, what non linear elements should be used, what operations should be performed digitally (if any). The design is an analogue for many of the physical and measurement principles underlying the study of reaction kinetics. It is very difficult to realise the specified functions if the analogue is simplified, or specialised, too early in the design process.

2.1.   Preliminary Background Information

Before starting the task, the subject knows he is to design an educational simulator for use in an A level chemistry course, based upon a mixture of the Nuffield Chemistry units on reaction mechanisms (topics 14, 15 and 17) and the Open University courses S100 (units 11 and 12) and ST28 (units 5 and 6) on reaction mechanisms and chemical equilibria. Extracts from these texts, which are very readable by people with a general scientific background, will be available.

In preliminary discussions, it should be possible to show the utility of demonstrations and simulations in education (there are plenty of well known examples) and to point out that this simulator must be peculiarly versatile if it is to cover the required experiments and allow for rational exploration of chemical system behaviours.   A list of experiments and situations is being prepared for preliminary reading.

2.2.   Environment

The designer is allowed ample bench space and has access to refreshments. He is provided with a small scale drawing board, pencils, pens and a "Sinclair Scientific" calculator capable of performing most of the calculations likely to be required.

In the same area there is a catalogue of component data sheets and facilities for constructing "breadboard" versions of simulator designs. A range of passive components, operational amplifiers, analogue multipliers and digital logic devices are available.

In order to suggest the possibility of unconventional solutions of the design problem, a number of less familiar non linear devices are available, notably, thermistors and FETs. The designer is allowed to ask for any other components he wishes, within reasonable limits upon cost and availability. Display devices (meters, an oscilloscope, digital display units, LEDs) are held in stock, since some of them are required in any design. Others can be ordered and made available at the next experimental session, provided they appear in the R.S. Components catalogue (R.S. Components is a supplier able to give rapid delivery of small quantities of a wide range of electronic components).

The components available are listed and indexed. Each component is given a realistic cost per 1, per 50, per 100, per 1000 batch.

2.3.   Scheduling

The design activity is meant to take place chiefly in the laboratory, during a series of personally arranged sessions. All original notes are held in file, though photocopies are provided.

If a designer does paper and pencil work outside the laboratory, he is asked to estimate the time spent and to say what progress he made, at the next experimental session. The length of a session is not rigidly fixed, apart from stipulating that half an hour must be allowed at the end of each session for analysis. Analysis includes

objective recording of the work done during the session and takes place in an adjacent room where the tutorial facilities for Group B students, and the analytical facilities for all students are situated.

2.4.   Aim or Objective

A design consists of

(a) a circuit specification
(b) a working unit which satisfies this specification.

The task does not call for excessive wiring up of circuits and no real skill difficulty is anticipated. The large number of components is needed to allow latitude of design and not because an actual design is likely to be made up from large numbers of small parts. In any case, a technician will be in attendance to help with manual skills, pin recognition and other quite trivial problems.

2.5.   Interrogation of the Circuit Designer

During the body of a session the interrogation is informal and, so far as possible, the experimenter plays the role of a colleague. The 2 experimenters available are both knowledgeable designers, and will each have carried out the design task. Each stage in the design is recorded and the reasons given verbally, for designing in a particular way, are tape recorded. In the objective analysis phase, which terminates each session, mechanical/electronic procedures are employed and inevitably formalise the interrogation. But, even at this point, the experimenter will be present to give help.

The term "analysis" has a precise meaning. The current design is regarded as though it were a theory or hypothesis and the designer is regarded as though he were a course author expounding his "theory" about topics in an academic, or technical subject matter. He is asked "how" and "why" questions about each part of his design, using the partly automated and computer monitored technique noted in the proposal. He is required to respond within a standard format. If at this stage, a circuit (even if only partially complete) is constructed, his response may include pointing at the equipment and demonstrating its behaviour, which is also recorded.

2.6.   Constraints Imposed upon the Design Task

The constraints noted in <u>Proposal</u>, Appendix A, Section 2.2.1. can all be interpreted in the context of the design task. These constraints are –

(a) Reliability
(b) Transparency – ease of fault detection or replacement of parts
(c) Weight/size/cost of the equipment
(d) Environmental sensitivity.

The meaning of these terms will be explained to subjects, together with the frank admission, that optimising with respect to one constraint does, as a rule, have an adverse effect upon performance with regard to other constraints. In view of this, a compromise design is quite acceptable. The first task design must be an inexpensive portable equipment (low weight/size/cost) and it should be reliable. To some extent, reliability depends upon environmental sensitivity which, in this case, is largely determined by the type of user display and control interface. Several interesting problems are posed, similar to those encountered with exhibition equipment, in order to render this inter-face foolproof. Although there is no question of vandalism, the equipment is to be used by groups of busy people.

Unit cost should be estimated as a function of ($\sqrt{}$component cost$\sqrt{}$ + $\sqrt{}$assembly technique$\sqrt{}$ + $\sqrt{}$labour, estimated per hand wired connection needed$\sqrt{}$) and is to be minimised subject to adequate functioning and high reliability or ruggedness. Unit cost should not exceed £150.

Tradeoff between versatility of the simulator, its reliability, and cost, are open to discussion. The subject has an opportunity to meet typical users, for example, science teachers, if in doubt.

2.7.   Specification of the Equipment: Design Brief

A designer is given the following specification and can ask any questions he wishes.

8

<u>Brief to Designer (Draft form currently being tested)</u>

The equipment is to be portable and rugged. It is typically used by small groups of 16 to 18 year old students in a chemical laboratory. It is to simulate the progress of a chemical reaction, by displaying the concentration (or, in some cases equivalently, the vapour pressure) of the reactants and products. The conditions under which the reaction occurs are partly prescribed by a program card (or similar device) inserted for a particular exercise, and partly by the control of the users.

The concentrations, are usually written, in chemistry as square bracketed terms.

For example $\angle Z \angle$ = concentration of Z.

Concentrations change over time from a resetable zero (t = 0). Concentrations are measured, so far as the simulator is concerned, on a scale 0 to 50, and to an accuracy of $\pm$ 1 in the centre region. The ends of the scale, are necessarily and inoffensively, inaccurate.

The absolute value of time in one simulated "run" is immaterial, apart from observability, and will probably depend upon your choice of components and display equipment. At any point, it should be possible to "freeze" the concentration values long enough to note and record them, without embarrassingly large drift. In practice, allow for no less than $\frac{1}{2}$ mins. observation as "apparently drift free".

As a general case, the simulator is to deal with a reaction involving reactant molecules A and B and product molecules C and D. The reaction is stoichiometrically (ie molecular-chemical-formulation) characterised by an equation :

$$V_A A + V_B B = V_C C + V_D D \tag{1}$$

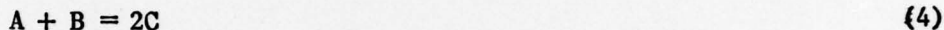where V_A, V_B, V_C and V_D are the "stoichiometric coefficients".

The equation may be rewritten :

$$V_C D + V_D D - V_A A - V_B B = 0 \qquad (2)$$

Replacing A, B etc. by a variable Z, the equation may be rewritten in its most general form :

$$\sum_Z V_Z Z = 0 \qquad (3)$$

The simulation should allow for the possibility that only one reactant or product may be involved. For example, the reaction :

$$A + B = 2C \qquad (4)$$

For which the stoichiometric coefficients are :

$$V_A = -1, \ V_B = -1, \ V_C = 2, \ V_D = 0$$

(using the standard sign convention)

Recalling that $\lfloor Z \rfloor$ stands for concentration. The rate of a reaction involving A, B, C, D is defined to be :

$$\text{Rate} (\lambda) = \frac{1}{V_Z} \ \frac{d \lfloor \bar{Z} \rfloor}{dt} \qquad (5)$$

with Z = A, B, C or D

For the reaction of equation (4) the rate is defined, therefore, as :

$$\lambda = \frac{-d \lfloor A \rfloor}{dt} \quad \text{or} \quad \frac{-d \lfloor B \rfloor}{dt} \quad \text{or} \quad \frac{1}{2} \frac{d \lfloor C \rfloor}{dt} \qquad (6)$$

Generally, the rate of reaction depends upon the concentration of the reactants, and the temperature at which the reaction takes place.

The simulator has to handle, as special cases :

(a) Reactions occurring at a constant temperature. Since chemical reactions are generally accompanied by energy changes manifest by the absorption or emission of heat, "constant" temperature" simulation involves representing a thermostatic device to maintain this condition.

(b) Reactions which take place at constant pressure. A "constant pressure" simulation involves representing a feedback device, similar in function to the thermostat which corresponds, in turn, to various contrivances that are used in experimental work to secure this condition for some or all of the reactants.

Since something has to be done in order to maintain either of the "special case" constancies, additional displays are required in order to show what is done.

For example, in the "constant temperature" case the heat change (signified Δ H, the enthalpy change) of the reaction must be compensated. If the reaction is exothermic (Δ H negative) the reaction vessel must be cooled, if the reaction is endothermic (Δ H positive) the reaction vessel must be heated. This heating or cooling action must be displayed when the "constant temperature" condition is involved in the simulated reaction. Similarly, to maintain the "constant pressure" condition it is usually necessary to bring reactants into the system and/or to remove reaction products. These operations must be clearly displayed.

Under constant temperature conditions reaction rate, λ , depends upon the concentrations of one or more reactants. The rate can be expressed as a function of the concentrations of the reactants and a constant, k, known as the "rate constant" for the reaction. For example :

$$\lambda = K [A] \tag{7}$$

$$\lambda = K [A] [B] \tag{8}$$

For example, referring to equations (4) and (6) the simulation requirements for a particular reaction may be specified by the equations :

$$\lambda = K [A] [B] \tag{9}$$

$$\lambda = \frac{-d[A]}{dt} = \frac{-d[B]}{dt} = \frac{1}{2}\frac{d[C]}{dt} \tag{10}$$

In general, the concentration terms in a rate expression appear as not–necessarily–integer valued powers. The general form of the rate expression for a reaction involving A, B as reactants is :

$$\lambda = K [A]^{U_A} [B]^{U_B} \tag{11}$$

The values of U_A and U_B being typically between 1.0 and 3.0.

When it is possible to express reaction rate by such equations (and it usually is, though the form of the expression depends upon the reaction mechanism) the sum of the exponents in the rate expression is termed "the order of the reaction".

$$\sum_Z U_Z = \text{Order of reaction} \tag{12}$$

For example the reaction governed by the rate equation of equation (8) has order 2, the reaction of equation (7) order 1 and so on.

You may restrict your design to reactions that can be given an order: if so, values between 1 and 3, accurate to $\pm$ 0.05 are required. You may also consider a more general scheme since users should recognise that reaction order only has meaning, if by knowledge of the mechanism concerned, or by empirical determination, it is possible to express the reaction rate in the form of equation (11). There are some reactions for which the concept of order is meaningless even though this concept is generally very useful as an abstraction.

If you are familiar with chemical notation, Table 1 provides examples of reactions with different orders and one having no meaningful order (ie the "order" abstraction is, in this case meaningless simply because the rate equation cannot be expressed in the form of equation (11)).

So far, it has been tacitly assumed that chemical reactions "go" in one direction and, consequently it was possible to make a distinction between reactants as "input" and products as "output". This assumption is sometimes _nearly_ "true" under some energetic conditions and at _some_ temperature.

For example, it is sometimes true that

$$A + B = 2C \tag{13}$$

means

$$A + B \rightarrow 2C \tag{14}$$
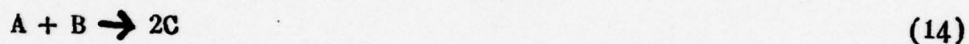
In general, the assumption is false. There is nearly always a significant back reaction under some energetic conditions and sometimes the reaction can only be usefully regarded as a dynamic equilibrium.

For example

$$A + B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} 2C \tag{15}$$

k_1 and k_2 denote the rate constants for the "forward" and "back" reactions respectively.

The ratio of concentrations at the dynamic equilibrium point is called an equilibrium constant K (for a given set of reactants at a given temperature).

$$K = \frac{[C][D]}{[A][B]} \quad \text{for } A + B \rightleftharpoons C + D \tag{16}$$

One point to be made by the tutorial use of the simulator is that though an expression for the equilibrium constant can be written as in equation (16) the rate constants cannot be written directly.

In the simulator, values of k_1, k_2, and the concentration terms into which they are multiplied will be coded, together with other reaction characterising parameters, on the program card (or any similar device employed). You must assume that a back reaction exists, unless the contrary is stipulated by data on the program card. When both forward and back reactions are present one reaction process may be dominant. Further, each process depends upon a distinct rate constant and may have a different order.

A design to meet this specification is (marginally) sufficient. However, in view of the complicated interactions possible in such a system, and the further complications that arise as the temperature is varied, or various reaction-promoting or catalytic agents are introduced, it may be wise to opt for a symmetrical design. In a symmetrical design the concentration of all 4 molecular species (A, B, C, D) are in a dynamic equilibrium, potentially interacting with each other. Normally the interactions are restricted by the constraints that are coded on the program card (for example, to the effect that only the concentrations of one species significantly influence the reaction between another pair, and so on).

A symmetrical design is a more accurate analogue provided that sufficient program data is encoded. It is also more elegant and, we suspect, easier to build when everything is taken into account. Notice, for example, that the reaction

$$A + B \rightleftharpoons 2C \tag{17}$$

is neatly converted into the special case of

$$A + B \rightarrow 2C \tag{18}$$
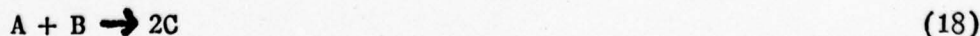
By applying the "constant concentration" regulator and setting $[C]$ near to zero (so that C molecules are "removed by the regulator

as they are created"), which ties up with real life conditions, where C molecules are removed or rendered inactive, perhaps because they form an insoluble precipitate.

The rate of reaction depends upon temperature often in an unsymmetrical manner. For example, $A + B \rightarrow 2C$ may be dominant at some temperatures $2C \rightarrow A + B$ at others. Fortunately, it is possible to build into the simulator a general principle (due to the chemist Arrhenius and others who developed the idea) relating the rate constant, k, to temperature, independently of the concentrations involved. This entirely general principle is

$$k = \alpha \, \mathrm{Exp} \, \frac{-\beta}{RT} \qquad (\text{or } \mathrm{Log}_e \, k = \mathrm{Log}_e \, \alpha \, \frac{-\beta}{RT}) \qquad (19)$$

In both equations α and β are specified as constants (one structural, the other energetic) for particular reactions, through the program card. You should allow values of α between 10^5 and 10^{10}; for β between 100 and 1000. R is the gas constant $8.314 \, \mathrm{KJ}^{-1}\mathrm{MOL}^{-1}$, and T is the absolute temperature. Only T is to be considered as a variable (albeit, held constant by your "thermostat" in the "constant temperature" condition). Values of T between $250^{\circ}K$ and $1000^{\circ}K$ should be allowed for, to be maintained with an accuracy of $\pm 20^{\circ}K$. Here, as noted before, a measure of compromise is possible and the precise range of values chosen for the design may be discussed.

Without prejudicing the design adopted it may be helpful to indicate one layout using meter displays. This layout is shown in Fig 2.

The meters read the concentrations $[A]$, $[B]$, $[C]$, $[D]$ as they change throughout the simulated interval. The signal lamps indicate whether a meter is or is not in use. For example, in a reaction involving only a single product (C) the meter displaying the concentration of product D is not in use. Similarly in a tutorial exercise, where a concentration is to be determined, one meter would not be in use. The same meter/lamp convention is used for the other display meters.

The dials give initial concentrations denoted $[A]_0$, $[B]_0$, $[C]_0$, $[D]_0$. Constant temperature or pressure conditions are set also by turning dials and operating associated switches. The meter T shows the temperature of the reaction vessel (assumed to be of a standard size) and the dial indicates either an initial value T_0, or (under the constant temperature condition) a constant value.

The thermostatic work meter TW is activated only in the constant temperature condition and shows the heating or cooling needed to maintain the constancy in question.

The concentration work meter, CW, is activated only if one or more of the concentrations is held constant and shows the introduction or removal of a reactant or product.

The start button initialises the simulator, at the preset initial concentrations and preset temperature value. The stop button puts the simulator into a "hold" condition.

The program card carries coded information which may include initial conditions or not, but which does include critical data (rate constants, α, β, values of exponents in the rate expression). The program data may also include information concerning a further component, not mentioned so far, namely, the presence of a specific catalyst, or of products that act as autocatalytic agents.

For tutorial purposes these inputs may be regarded as establishing: (a) the rate equations for both forward and back reactions (b) the values of the variables (α and β) in the Arrhenius equations determining the relationship between rate constants and temperature.

Unless the constant temperature condition prevails the temperature is computed using :

$$T_n = T_0 + \int_{t=0}^{t=n} F \text{ (concentrations of reactants) } dt \qquad (20)$$

F is given, as a table, in the program data: it condenses information about heat of reaction assuming that the thermal capacity and volume of the system are constants and known.

2.8. Evaluation of the Design

Complete records, from the objective analysis and the experimenter/ subject interaction, are available and contribute the main data. However, the following evaluations are possible, at the end of the first design task, and do, at least, provide motivating feedback.

(a) Does the simulator submitted do everything it is supposed to do?

(b) How is it judged by expert designers (Group A subjects) in terms of its function and the compromise achieved between reliability, transparency, weight/size/cost and environmental sensitivity.

(c) Any team of 4 or 5 subjects starting the second design task bring with them 4 or 5 simulator designs and bench mock ups. As noted in Section 1.3 the second task incorporates a simulator, with the first task specification as one subsystem. It seems likely that one of the simulations already designed will be selected. At any rate, the teams of 4 or 5 subjects have an opportunity to make such a selection and it should, therefore, be possible to obtain an index of peer group evaluation.

3. The Second Design Task

Teams of 4 or 5 subjects tackle the second design task, outlined in Section 1.3. Some teams will consist of both Group A and Group B subjects, other teams of student designers on their own. During the first design task all subjects have been exposed to the background material (referred to in Section 2.1), so that the reasons for building a larger simulator should be evident.

3.1. Differences Between First and Second Design Tasks

(a) The first design task is carried out on an individual basis. The experimenter acts as a colleague (and if need be an assistant). The second task is a team activity for two reasons; the design is complex enough to require concerted action and division of labour; the team situation is deliberately contrived to exteriorise communication between designers. The experimenter is chiefly concerned with promoting useful discussion which is tape recorded.

(b) As before, the team meets at personally arranged sessions (provided that there are no regular absentees, it should not matter too much if some members are occasionally unable to attend a session). It is impracticable to carry out a design analysis for each individual at each session (as in the first task). Each individual will, however, have his concept of the team design analysed once during the series of sessions. All individuals will submit to analysis of this kind when the design is "finished". As noted in Section 1.3, the second task can be terminated at various stages. How far a team proceeds will depend upon practical possibility and the yield of relevant data.

(c) The team working environment will be either a discussion room, or the laboratory, as desired. The bench equipment used, at the laboratory, in the first design task is augmented by our minicomputer which has unusually liberal interfacing capabilities. For example, there are analogue/digital converters and a general I/O bus system to which a (practically unlimited) number of devices may be attached.

The computer may be used to couple hybrid or analogue networks (similar to those of the first design) or to organise display sequences. This expedient is satisfactory for design purposes, however, the subjects are told (truthfully) that a practical simulator for use in a classroom would have to implement programmed instructions using a dedicated microprocessor; ie it must be "brought in" and "switched on", like any other piece of laboratory equipment, if it is to be used in real life.

(d) The design specification (discussed below, in Section 3.2) is a set of guidelines for demonstrating as many of the physical and chemical principles in the background materials as possible.

(e) The constraints upon the second design differ from the constraints involved in the first design task. Provided the simulator is transportable, its size and weight are not critical. The cost may be as much as £1,000, since the simulator would typically be used by several schools. Reliability is important, but, because the simulator is complex, transparency is even more so. A laboratory technician (not usually an electronics technician) should be able, after instruction, to identify and replace any defective modules. Since the simulator will be used under supervision, environmental sensitivity (with the meaning acquired during the first design) is not a primary consideration, though obviously the simulator should be as insensitive as possible to misuse.

3.2.   Design Specification

Background materials apart, the design guidelines are verbally indicated by the experimenter. The following comments highlight salient points which the experimenter will stress and, where necessary, explain.

Two related types of demonstration are desirable. One simulating the mechanisms of chemical reaction, the other illustrating the energy exchanges which occur during a reaction.

According to the background materials, concepts of reaction mechanisms are developed from the starting point of the simple

collision model, ie that molecules react if they collide and if their kinetic energy is large enough to "break" certain (covalent) bonds. However, this model does not check out at all well empirically, for several reasons.

To begin with, several counterfactual assumptions are built into the elementary methods of estimating collision frequency; for example, that molecules have "no volume" (they are "points"). Even if this assumption is replaced by a more realistic assumption, that molecules do occupy a volume, the results still do not fit the facts very well. A better empirical verification is achieved if the molecular energy is considered as made up of kinetic + vibrational + potential energy. Potentially reacting molecules in close proximity are regarded as vibrational oscillators, able to exchange energy through a resonance mechanism which depends on the relative vibrational frequencies, transit time and relaxation time.

Models such as this are the most sophisticated to be simulated (though they are not the most sophisticated models that exist). They still provide inadequate predictions unless it is recognised that few, if any, reactions proceed by direct paths, (a point which is taken up very soon).

So far, it would be necessary to display the motion of "point molecules" as a function of temperature (using Boltzmann's Distribution, as in Fig 3); the motion of "finite volume molecules", and the phenomenon of resonance. The latter is to be displayed (Fig 4) by locating an observer on one molecule and showing (relative to this one molecule) the spatial motion of other labelled molecules. Vibrational frequencies may either be displayed visually, or as the amplitude of tone coded audio signals.

The experimenter now returns to the notion of a reaction path, and through this to the energetic considerations. As is evident from the background materials, chemists draw pictures relating the energy of a system to its position on a "reaction co-ordinate". The sketches in Fig 5a and 5b are fairly typical.

It is necessary to explain (if possible, by a graphic simulation) that the "reaction co-ordinate" is, in fact, a minimum potential energy surface, representing the minimal configurational energy of a reacting system. This fact can be illustrated by a 3 dimensional figure only for unrealistically simple reactions. Though this demonstration proves extremely useful (Fig 6, taken from S100 Unit 11) an animated (possibly colour) display might do even more.

Next it is necessary to explain that E (in Figs 5 and 6) is the energy of a particular reacting system under consideration, and that the hump (M) is the energy level above which reaction can take place between adjacent molecules of the reactants. The concepts of the energy of the reaction system, and the "energy barrier" (M) should, therefore, be incorporated in the simulation.

Finally, Δ H in the sketched pictures is the enthalpy of the reaction, as noted in Section 2 but with a definition refined as follows :

For a reaction carried out at a constant temperature (T) and at a constant pressure, the enthalpy change for the reaction is :

Δ H (at temp.T) = "The amount of heating or cooling done by a thermostat in order to compensate for either (a) heat absorption by an endothermic reaction (in bond formation) or (b) the heat emitted in an exothermic reaction (by bond breaking).

If the reaction is carried out under "standard conditions" (usually one atmosphere pressure with the reactants in the states normal for the temperature being used) the enthalpy change obtained is the "standard enthalpy" for the reaction. The standard enthalpy is usually denoted as $\Delta H^{\ominus}(T^{0}K)$.

Both exothermic and endothermic energy exchanges can be demonstrated using the first simulator.

One determinant of whether or not reactions occur is energetic, but the other is structural. In considering the structural component, it becomes clear that there are usually many reaction mechanisms which can be depicted in the framework of the reaction co-ordinate/energy pictures. The sketches in Fig 7a, Fig 7b and Fig 7c illustrate this point. As a special case there is the notion of a "highest energy" activated complex of molecules that breaks down into products in stages (as shown in Fig 7c).

One simulator for such processes would consist of several of the simulators built for the first design task coupled together, in series or in parallel, augmented by an appropriately transformed state display (Fig 8).

Various other simulation possibilities exist. Of particular interest is the relationship between Free Energy Change ΔG, Temperature, entropy change ΔS, and enthalpy.

$$\Delta G = \Delta H - T \Delta S \quad \text{or} \quad \Delta G^{\ominus} = \Delta H^{\ominus} - T \Delta S^{\ominus} \tag{20}$$

also the relationship between the equilibrium constant K, of Section 2, the standard enthalpy, and temperature.

$$\frac{d \, \text{Log}_e \, K}{dT} = \frac{\Delta H^{\ominus}}{RT^2} \tag{21}$$

As noted (Section 1.3) it is intended to pursue these possibilities, all of them rich in analogies and suggesting ingenious and innovative design, as far as it seems experimentally profitable to do so.

4.   Comments Upon Computer Administered Tests

As noted in Section 1.1. computer programs for administering tests for cognitive style (for instance the "Spy Ring History Test") were completed during the reporting period. Table 2 shows in outline the operation of the Spy Ring History Test program.

Computer administered testing allows for the collection and use of information which it would be impracticable to obtain by mental test administration.

For example, confidence estimate responses are elicited over and above deterministic responses. All subjects are required to estimate the confidence (degree of belief) that a constructed response (such as a list or a graph or a map) is a correct response, and to provide confidence estimates (which may degenerate into all or none selections) over the choice alternatives of the multiple choice questions.

Such responses are known to be more informative for some subjects (those able to give reasonable estimates, or those who can rapidly learn to do so). The real value of the method lies, however, in situations where it is possible to calibrate the individual confidence estimates against an objective correct response index.

Calibration is obtained over the initial "memory loading" operation (Table 2) during which the subject learns the basic lists and their relations. He is required to learn each list to a criterion of one faultless repetition (the criterion can be changed very easily) but, in doing so, commonly submits a series of repetitions for each list, containing some mistakes. For each response submitted during the initial "loading" operation the subject gives an estimate that his response is entirely correct. It is thus quite easy to calibrate the confidence estimate with respect to an objective criterion (also stored) of how many correct items there really are in the response (Note – during the last rehearsal trial of the series all items are correct, using the present criterion). Further, this process is repeated for all 5 lists.

The calibration, so obtained, is used in evaluating confidence estimates with respect to the recall responses elicited later in the test.

Since 5 lists are learned it is also possible to compare the individual scores <u>within</u> repetitions of one list and <u>between</u> the lists of the series. As a result of this comparison an index of individual learning rate (finite difference score increments), an index of individual neutral score ("learning ability", in general) and an index of individual score variability are computed by the system.

These calibration figures and indices can be used by the experimenter, "off line", in order to assess the characteristics of the subject and, on averaging over an individual (pretest/ post-test), or a group of individuals, to enhance the statistic value/reliability of the data. A possible "on line" use of the indices, not yet implemented but known to be effective, is to guide adaptive test administration. One adaptively controllable variable is the correct score threshold; another, is the number of "points" charged, to access the original data base for items of information in order to bring recall scores up to a fixed criterial value.

5.   Training for Group B Subjects: the student designers

From the interviews carried out during the year, it seems that most subjects selected as student designers are likely to have a fair theoretical knowledge of the components to be used in the design task. In contrast, these subjects are not likely to have much practical experience or knowledge of system design skills. For example, predicting the behaviour of a system constructed from non ideal components, and making the necessary costs/performance tradeoff decisions for individual components in order to achieve the desired overall system performance.

This area of weakness is probably symptomatic of a general inability to see things as a whole and to examine similarities and differences between parts of the whole system.

Training will check subjects' familiarity with the basic components, any necessary instruction being given, but will be concentrated after that, upon (A) basic design principles and (B) the areas of weakness or ignorance already noted.

In view of recent findings (as yet, only mentioned in publications) which strongly indicate that subject matters for training should be represented from several (rather than one) perspective/point of view, it is prudent to use for training a general course assembly and tutorial system with this capability built into it.

The choice of training system is a tactical point and in no way modifies the basic experiment, since the training environment contains all of the facilities, noted in the Proposal Appendix A. Section 1.2., as subsystems. However, certain advantages are gained by this tactic, these are listed below.

(a) Training can be more flexible, and behavioural records (including those which exteriorise cognition) are more readily obtainable.

(b) The operating system (<u>Proposal</u> Appendix A, Section 2.5 (4)) should be more comprehensive than anticipated and, since more routines are incorporated in computer programs (rather than "hardware"), more readily "transferable".

(c) The "instructional materials" (<u>Proposal</u> Appendix A, Section 2.5 (6)), will be a systematic development of the original material generated over the entire experimental series.

6. Comments on Experimental Design.

It appears practicable to satisfy the goals set out in the proposal with only the following deviations from the original plan :

(a) To employ a first and a second design task, of which the second is of optional length and taps communication between designers in a team (Sections 2 and 3). The second task could probably be justified as a means of eliciting communication (verbal co-operation, etc.) without adulterating the (closely monitored) individual records from the first task. However, the second task can also be justified as a means of "interviewing" subjects in the context of the first design. In addition, the broader context provides a realistic framework in which subjects are likely to see the first simulator design as a "meaningful", rather than a merely academic, exercise.

(b) To use a general operating system for training sessions with Group B subjects (this does not influence the experimental philosophy and the advantages were outlined in Section 5).

(c) To introduce pre-test and post-test measures of versatility (one of the variables scored in the Spy Ring History Test, for Learning Style) and to examine the effect of specific versatility training (Proposal, Section 2(b)) upon pre-test/post-test scores and upon designer/student designer performance. The intention is to concentrate specific versatility training in the analysis parts of the sessions.

The overall experimental design is summarised in Table 3.

1st Order	$C_2 H_5 Cl = C_2 H_4 + Cl$ $$\lambda = k [C_2 H_5 Cl]$$
2nd Order	$H_2 + I_2 = 2\ HI$ $$\lambda = k [H_2] [I_2]$$
Higher integral order	$2\ NO + O_2 = 2\ NO_2$ $$\lambda = k [NO]^2 [O_2]$$
Other-than-integral Order	$C_2 H_5 B_r = C_2 H_4 + HBr$ where $\lambda = k [C_2 H_5 Br]^{1.5}$
No meaningful order	$H_2 + Br_2 = 2\ HBr$ (no meaning because reaction rate has the form $$\lambda = \frac{k_1 [H_2] [Br_2]^{0.5}}{1 + k_2 [Hr_2] / [Br_2]}$$

Table 1.   Reactions of different order for comparison by designers who are familiar with chemical notation (an optional but, in view of a science background, likely expertise). Gas reactions are used to unify the presentation.

(1) Display list 1; pre-determined inverval. Display graph.

(2) Request subject reproduce list. Record score.

(3) Elicit confidence estimate. Subject positions cursor along illuminated bar on screen. Record % with score from (2).

(4) If score (2) not satisfactory repeat (1) – (3) until criterion satisfied. (All scores/confidence estimates recorded).

(5) Repeat procedure (1) through (4) for lists 2 through 5. All scores tagged for print-out.

(6) Display information points. Initially 50.

(7) Request map of three countries. If response within allowed time go to step (9) otherwise carry on at (8).

(8) Offer information menu and display chosen item(s). Dip motivation points appropriately. Go back to (7).

(9) Get confidence estimate. If map correct carry on otherwise go back to (8).

(10) Repeat (7) through (9) but request spy positions within countries.

(11) Prediction test (1981) Display map with spies in correct countries. Request links between spies. Repeat procedure as in (7) through (9).

(12) Request recall of lists and networks for all years. (Lists or networks first).

(13) Lists can be recalled as learned or as representative sequence of any reasonable length. Record all responses.

(14) Networks recalled as maps showing countries or as abstract graphs (subject can do both). Record all responses.

(15) Final scoring.

Style pretest (including versatility)	Design Training	1st Design task (several sessions) Individual behaviour	2nd Design Task. (several sessions) Team behaviour	Styles Post test (including versatility)
Group A Group B	Group B	Group A + Group A − Group B + Group B −	Mixed team + Mixed team − B Team + B Team −	Group A + Group A − Group B + Group B −
Computer recorded test data and analysis of results.	Training data. learning strategy used. Learning Strategy effectiveness.	Computer recorded analysis data for each session and behavioural record. 1st Design evaluation.	Computer recorded analysis data for 2 sessions per individual in team. Record of team discussion. Informal 2nd Design Evaluation.	Computer recorded test data and analysis performed in context of results obtained at the earlier stages in experiment.

Table 3: Overall design of the experiment. Subjects given specific versatility training are marked by a "+" and those not given versatility training by a "−". Group A experienced designers. Group B student designers. The uppermost row of the table shows sequence of events, the middle row the composition of subject sample experiencing tests, training etc., the lowermost row, the data to be obtained and recorded at each stage in the experiment.
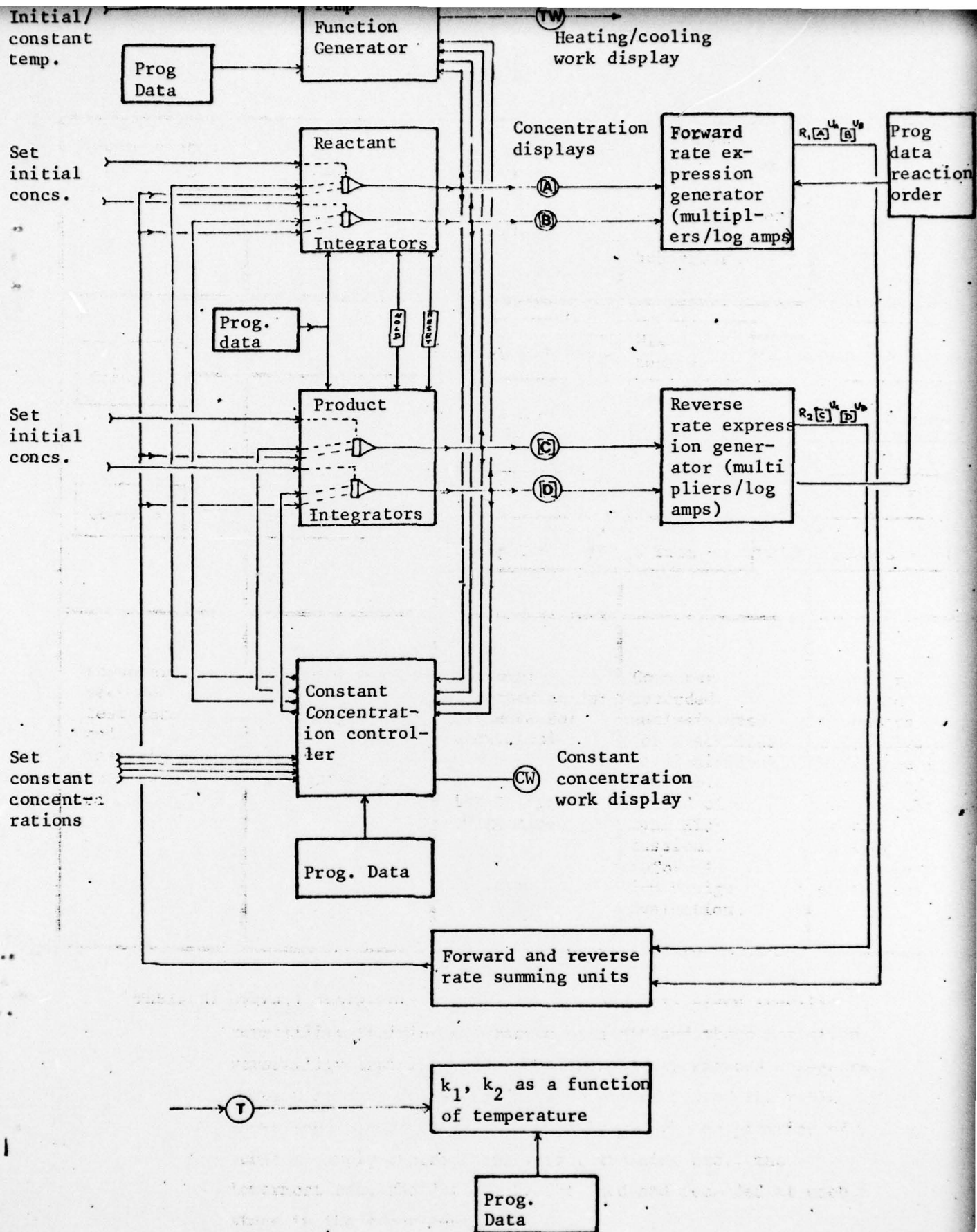
Fig 1:   An Outline Design for Reaction Simulator.
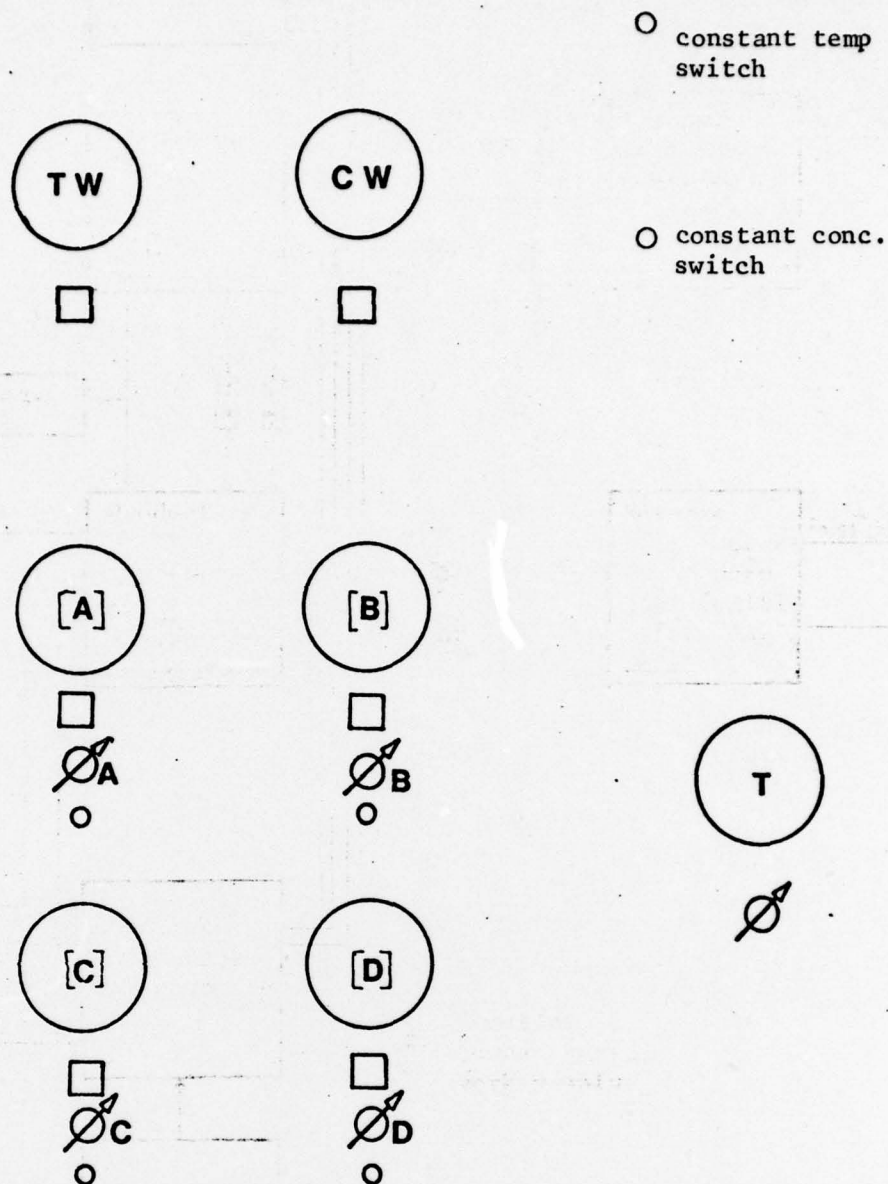
Fig 2. Possible display; ◯ meters; ▢ signal lamps; ∅
potentiometers as input "dials" for setting initial
or constant values of (A), (B), (C), (D) as determined
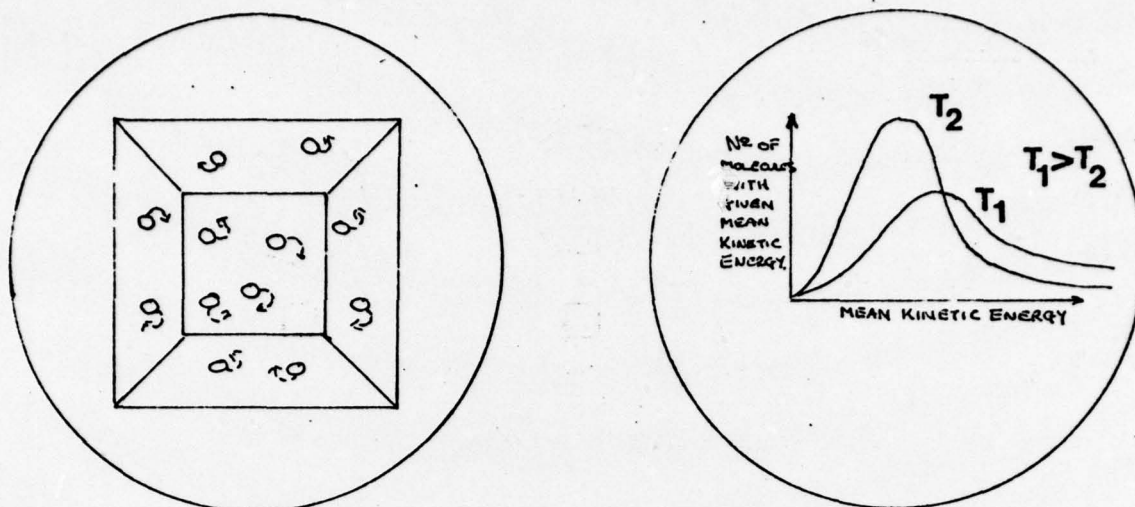by the switches ○, and setting initial or constant
temperature.

Fig 3: Displays (probably on tube) required (left) for showing
motion of closed system of molecules as temperature is
varied manually and (right) distribution of mean kinetic
energy of molecules as a function of manually adjusted
temperature . Two values of temperature shown.
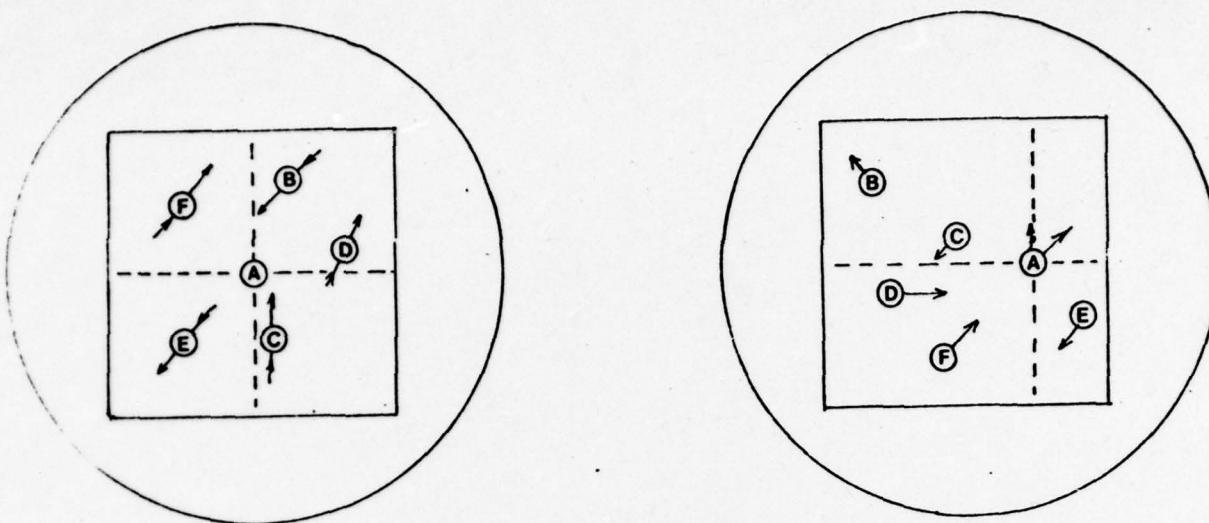
Fig 4:   Resonance display (left). Observer's coordinate system
moves with one (moving) molecule labelled A. Motions of
other molecules, B, C, D, E, are relative motions.
To stress that A is a moving point, it must also be poss-
ible to compare display with fixed reference frame (right)
where A, B, ... and grid lines centred on A all move
In (left side) moving frame of reference, display, A (though
actually in continual motion) remains fixed on the
screen as the observer's vantage point.

E

M

ΔH

a

reaction coordinate
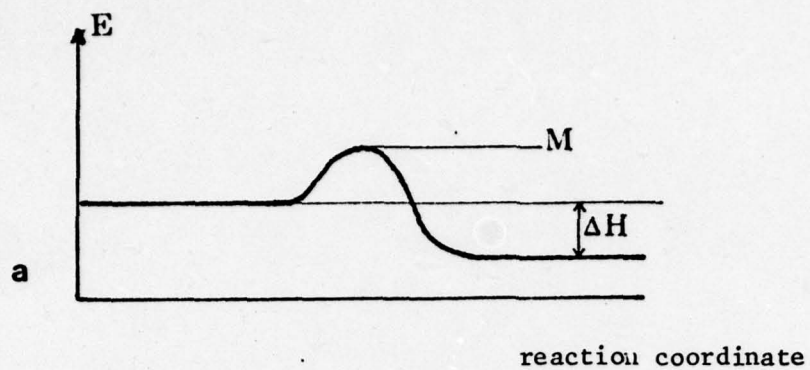
Exothermic reaction ($\Delta H < 0$)

E

M

ΔH

b
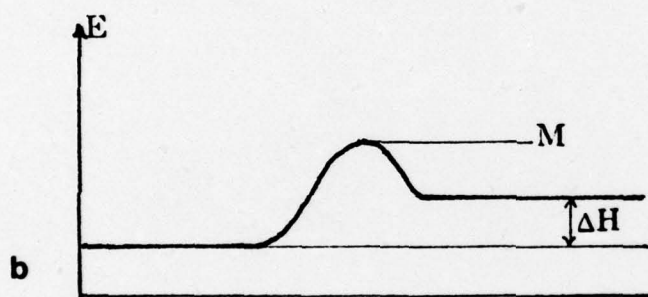
Endothermic reaction ($\Delta H > 0$)

Fig 5: Reaction coordinate/Energy Graphs
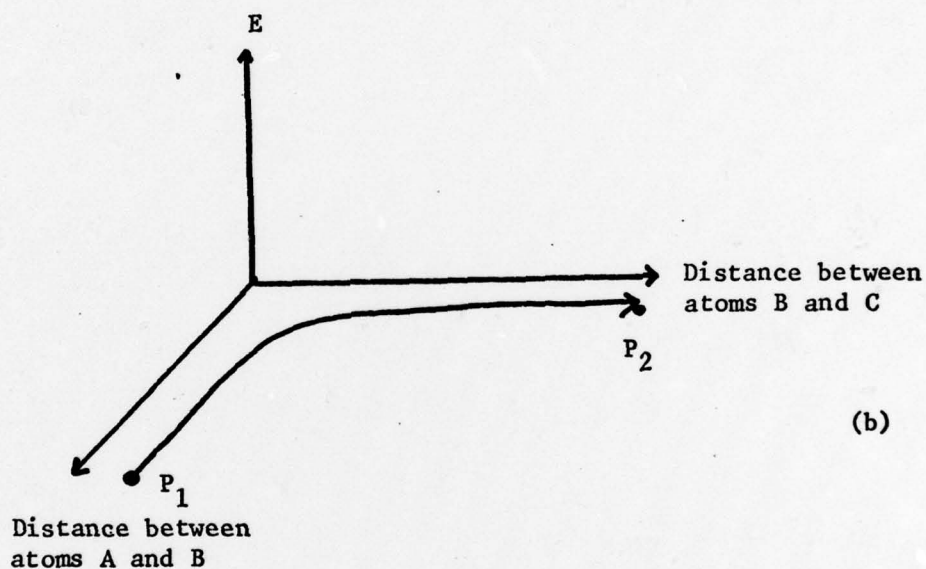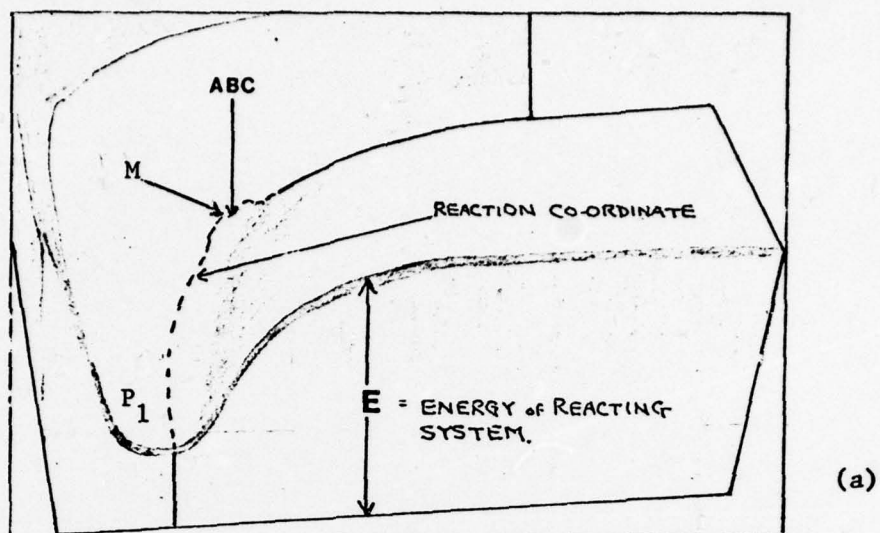
Fig 6: Sketch of a 3-dimensional model of the potential energy surface for a reaction between a diatomic and a monatomic molecule.

$$A + BC \rightarrow AB + C$$

The potential energy surface is shown for the atom A approaching B C along the line B C. Interatomic distances before the reaction takes place are represented by P_1 and after the reaction by P_2.
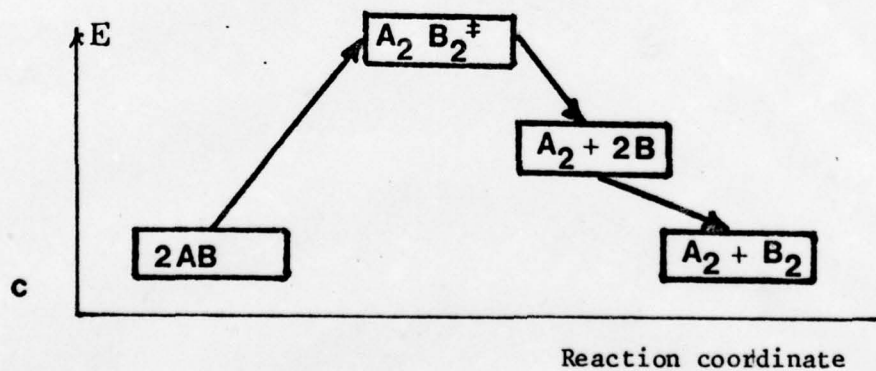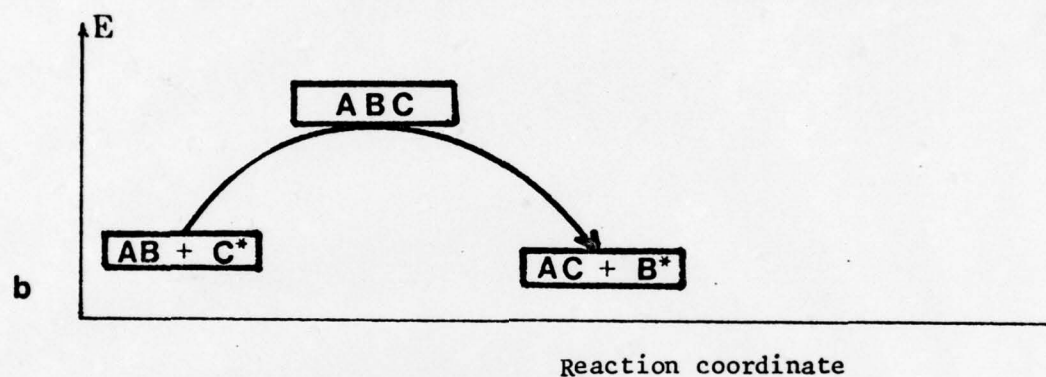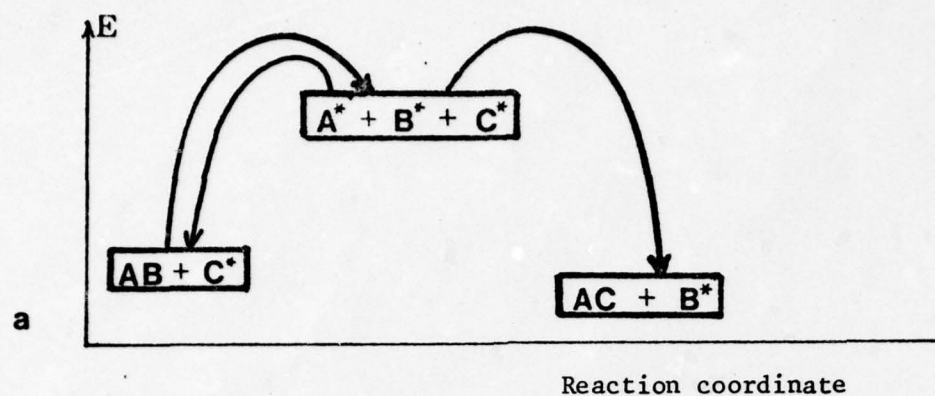
Fig 7: 7(a) and 7(b) show alternative reaction paths for the hydrolysis of bromoalkanes (*denotes an ionised molecule) 7(c) shows a reaction path (for the decomposition of hydrogen iodide) involving an activated complex (denoted ‡)
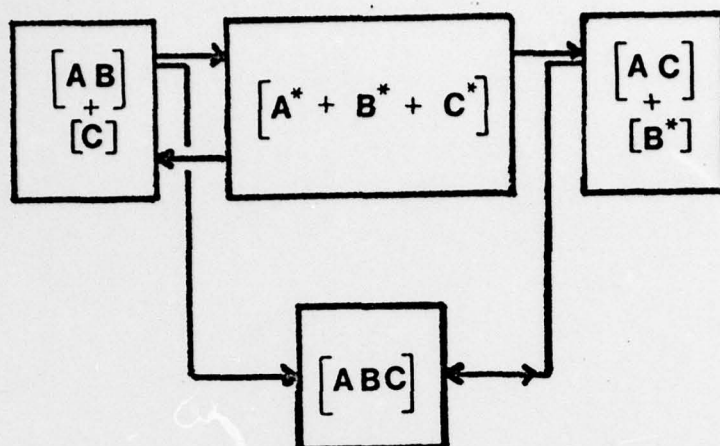
Fig 8: Parallel and series arrangement of Task 1 simulators
to show alternative reaction paths and a series of
reaction steps.

(Note: Apart from coupling, the trick is to notice
that, for any reaction, $\Delta H^{\ominus}$ is constant for all
reaction paths so that thermostatic and concentration
feedback loops around unit simulations are constrained
to be in register).